

# Spectral Methods for Numerical Relativity. The Initial Data Problem

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Numerical relativity has traditionally been pursued via finite differencing. Here we explore pseudospectral collocation (PSC) as an alternative to finite differencing, focusing particularly on the solution of the Hamiltonian constraint — an elliptic partial differential equation — for a black hole spacetime with angular momentum and for a black hole spacetime superposed with gravitational radiation. In PSC, an approximate solution, generally expressed as a sum over a set of orthogonal basis functions (e.g., Chebyshev polynomials), is substituted into the exact system of equations and the residual minimized. For systems with analytic solutions the approximate solutions converge upon the exact solution exponentially as the number of basis functions is increased. Consequently, PSC has a high computational efficiency: for solutions of even modest accuracy we find that PSC is substantially more efficient, as measured by either execution time or memory required, than finite differencing; furthermore, these savings increase rapidly with increasing accuracy.

For example, investigating the Hamiltonian constraint equation for a black hole with angular momentum we find that, where finite difference solutions require a resolution of  $1024 \times 384$  (radial  $\times$  angular) grid points to find a solution of fractional error  $10^{-5}$  in the ADM mass, a PSC solution achieves the same accuracy with only  $12 \times 4$  collocation points. Furthermore, the fractional error is reduced to  $10^{-10}$  by increasing the PSC resolution to  $24 \times 8$ , while the same increase in the finite difference solution would require (if it were possible) an increase in resolution by a factor of 300 in each dimension. Commensurate with the doubling of the resolution in each of the two dimensions the computing time required to find the spectral solution increase by a factor of  $2^2$  while the computing time required by the finite difference method would increase by a factor of  $300^2$ , or  $10^5$ .

The solution provided by PSC is an analytic function given everywhere, not just at the collocation points. Consequently, no interpolation operators need to be defined to determine the function values at intermediate points and no special arrangements need to be made to evaluate the solution or its derivatives on the boundaries. Since the practice of numerical relativity by finite differencing has been, and continues to be, hampered by both high computational resource demands and the difficulty of formulating acceptable finite difference alternatives to the analytic boundary conditions, PSC should be further pursued as an alternative way of formulating the computational problem of finding numerical solutions to the field equations of general relativity.

## I. INTRODUCTION AND SUMMARY

The partial differential equations (PDE) of numerical relativity have typically been solved using finite difference methods. In finite differencing (FD) one first chooses a finite number of coordinate “grid” points  $x_n$  and approximates the space and time derivatives in the PDEs by ratios of differences between field and coordinate values on the grid. With a choice of grid and “differencing scheme” for converting derivatives to ratios of differences, the equations of general relativity are approximated by a system of algebraic equations whose solution approximates that of the underlying PDEs.

In this paper we explore an alternative method for solving the elliptic PDEs encountered in numerical relativity: pseudospectral collocation (PSC). In PSC one begins by postulating an approximate solution, generally as a sum over some finite basis of polynomials or trigonometric

functions. The coefficients in the sum are determined by requiring that the residual error, obtained by substituting the approximate solution into the exact PDEs, is minimized in some suitable sense. Thus, if one describes FD as finding the exact solution to an approximate system of equations, one can describe PSC as finding an approximate solution to the exact equations.

Pseudospectral collocation has been applied successfully to solve problems in many fields, including fluid dynamics, meteorology, seismology, and relativistic astrophysics (cf. [1–4]). Its advantage over FD arises for problems with smooth solutions, where the approximate solution obtained using PSC converges on the actual solution *exponentially* as the number of basis functions is increased. The approximate FD solution, on the other hand, never converges faster than algebraically with the number of grid points. While the computational cost per “degree of freedom” — basis functions for PSC, grid points for FD — is higher for PSC than for FD, the com-

putational cost of a high accuracy PSC solution is a small fraction of the cost of an equivalent FD solution. Even for problems in which only modest accuracy is needed, PSC generally results in a significant computational savings in both memory and time compared to FD, especially for multidimensional problems.

The elliptic equations of interest here are the constraint equations that must be solved as part of the general relativistic Cauchy initial data problem. We focus on two axisymmetric problems: the initial data for a black hole spacetime with angular momentum, and a spacetime with a black hole superposed with gravitational waves (Brill waves). Solutions for both of these problems have been found by others using FD [5–7]: our focus here is to demonstrate the use of PSC for these problems and compare the computational cost of high accuracy solutions obtained using both PSC and FD.

In section II we review briefly the key constraint equations that arise in the traditional space-plus-time decomposition of the Einstein field equations and describe three different elliptic problems — a nonlinear model problem whose analytic solution is known, the nonlinear Hamiltonian constraint equation for an axisymmetric black hole spacetime with angular momentum, and the Hamiltonian constraint equation for a spacetime with a black hole superposed with Brill waves — that have been solved using FD and that we solve here using PSC. We describe PSC in section III, and compare the computational cost of PSC and FD for high accuracy solutions in section IV. In section V we solve the problems described in section II using PSC and compare the performance of PSC with that obtained by other authors using FD. In section VI, we discuss our conclusions and their implications for solving problems in numerical relativity. Finally, whether by FD or PSC the solution of a nonlinear elliptic system involves solving a potentially large system of (nonlinear) algebraic equations. We describe the methods we use for solving them in appendix A.

## II. INITIAL VALUE EQUATIONS

### A. Introduction

The general relativistic Cauchy initial value problem requires that we specify the metric and extrinsic curvature of a three-dimensional spacelike hypersurface. These quantities cannot be specified arbitrarily: rather they must satisfy a set of constraint equations, which are a subset of the Einstein field equations. Arnowitt, Deser, and Misner (ADM) [8] were the first to formulate the Cauchy initial value problem in relativity in this way; however, the most common expression of this 3 + 1 decomposition is due to York [9].

In the York formulation of the ADM equations the spacelike hypersurfaces are taken to be level surfaces of

some spacetime scalar function  $\tau$ . The generalized coordinates and conjugate momentum are the three-metric  $\gamma_{ij}$  induced on the spacelike hypersurface by the spacetime metric and the extrinsic curvature  $K_{ij}$  of the spacelike hypersurface.\* Position on each surface is described by a set of spatial coordinates  $x_i$  (where Latin indices run from 1 to 3 and indicate spatial coordinates on the slice), so that the line-element on the hypersurface is

$${}^{(3)}ds^2 = \gamma_{ij} dx^i dx^j. \quad (2.1)$$

The normal  $\mathbf{n}$  to the spacelike hypersurface is everywhere timelike. The time coordinate direction  $\mathbf{t}$ , however, need not be exactly along the normal. We can write  $\mathbf{t}$  in terms of  $\mathbf{n}$  and the spatial vectors that span the tangent space of the hypersurface:

$$\mathbf{t} = \alpha \mathbf{n} + \beta^i \frac{\partial}{\partial x^i}, \quad (2.2)$$

where the *lapse*  $\alpha$  describes how rapidly time elapses as one moves along the hypersurface normal  $\mathbf{n}$ , and the *shift*

$$\vec{\beta} = \beta^i \frac{\partial}{\partial x^i}, \quad (2.3)$$

is a vector field confined entirely to the hypersurface tangent space that describes how the spatial coordinates are shifted, relative to  $\mathbf{n}$ , as one moves from one hypersurface to the next. The lapse and shift are free functions: they correspond to the freedom to specify the evolution of the coordinate system that labels points in spacetime.

The *space-time* line element at any point on a hypersurface is related to the spatial metric at that point, the lapse, and the shift:

$$\begin{aligned} ds^2 &= g_{\mu\nu} dx^\mu dx^\nu \\ &= -(\alpha^2 - \beta_a \beta^a) dt^2 + 2\beta_i dx^i dt + \gamma_{ij} dx^i dx^j \end{aligned} \quad (2.4)$$

(where Greek indices run from 0 to 3 and include the time coordinate  $t$ , which is sometimes referred to as  $x_0$ ).

Given a spacetime foliation, choice of “field variables”  $\gamma_{ij}$  and  $K_{ij}$ , and coordinates (embodied in the lapse and shift), the field equations can be decomposed into four *constraint equations*, which  $\gamma_{ij}$  and  $K_{ij}$  must satisfy on each slice, and six *evolution equations*, which describe

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\*This approach is by no means unique. For example, recent work by Choquet-Bruhat, York and collaborators (cf. [10] and references therein) on a different choice of generalized coordinates and momenta have yielded approaches in which the evolution equations form a first-order symmetric and hyperbolic (FOSH) system. Many powerful numerical methods for solving FOSH systems exist and the numerical relativity community is only now beginning to explore how these solution techniques can be brought to bear on the field equations in this form.

how the three-metric and extrinsic curvature evolve from one slice to the next. In this paper we consider only the problem of consistent specification of initial data: *i.e.*, the solution of the constraint equations.

The four constraint equations (in vacuum) are

$${}^{(3)}R + K^2 - K_{ab}K^{ab} = 0, \quad (2.5a)$$

$${}^{(3)}\nabla_a (K^{ia} - K\gamma^{ia}) = 0, \quad (2.5b)$$

where  ${}^{(3)}R$  is the Ricci scalar associated with  $\gamma_{ij}$ ,  ${}^{(3)}\nabla_a$  is the covariant derivative associated with  $\gamma_{ij}$ , and

$$K := K_{ab}\gamma^{ab}, \quad (2.6)$$

is the trace of the extrinsic curvature  $K_{ij}$ . Note that, as befits constraints, equations 2.5 involve only derivatives of  $\gamma_{ij}$  and  $K_{ij}$  in the tangent space of the corresponding hypersurface.

## B. Conformal imaging formalism

Our goal is to determine a  $\gamma_{ij}$  and a  $K_{ij}$  that satisfy the constraint equations and boundary conditions. These are both symmetric tensors on a three-dimensional hypersurface; consequently, between the two there are twelve functions that must be specified. Equations 2.5 place only four constraints on these twelve functions. In order to solve the initial value problem, the remaining components of  $\gamma_{ij}$  and  $K_{ij}$  must be specified. York [9] has developed a convenient formalism, referred to as *conformal imaging*, for dividing the spatial metric and extrinsic curvature into constrained and unconstrained parts, which we summarize in this subsection.

Associate  $\gamma_{ij}$  with a *conformal background three-metric*  $\bar{\gamma}_{ij}$  through a *conformal factor*  $\psi$ :

$$\gamma_{ij} = \psi^4 \bar{\gamma}_{ij}. \quad (2.7)$$

The extrinsic curvature  $K^{ij}$  is split into its trace  $K$  and its trace-free part

$$A^{ij} = K^{ij} - \frac{1}{3}\gamma^{ij}K. \quad (2.8)$$

The trace  $K$  is treated as a given scalar function which will be specified. The trace-free extrinsic curvature  $\bar{A}^{ij}$  of the conformal metric  $\bar{\gamma}_{ij}$  can be expressed in terms of  $\psi$  and  $A^{ij}$ :

$$\bar{A}^{ij} = \psi^{10} A^{ij}. \quad (2.9)$$

The constraint equations (eqs. 2.5) can also be expressed in terms of the conformal background metric and its trace-free extrinsic curvature:

$$\bar{\nabla}^2 \psi - \frac{1}{8}\bar{R}\psi - \frac{1}{12}K^2\psi^5 + \frac{1}{8}\bar{A}_{ab}\bar{A}^{ab}\psi^{-7} = 0, \quad (2.10a)$$

$$\bar{\nabla}_a \bar{A}^{ia} - \frac{2}{3}\psi^6 \bar{\gamma}^{ia} \bar{\nabla}_a K = 0, \quad (2.10b)$$

where  ${}^{(3)}\bar{\nabla}_i$  is the covariant derivative associated with  $\bar{\gamma}_{ij}$ . Equation 2.10a is generally referred to as the Hamiltonian constraint, while equations 2.10b are generally referred to as the momentum constraints. Since the only derivatives of  $\bar{A}_{ij}$  appear in the combination of a divergence, only the longitudinal part of  $\bar{A}_{ij}$  is constrained by the momentum constraints.

Now turn to the boundary conditions. We are interested in problems with a single black hole. Let the initial hypersurface be asymptotically flat, so that on the hypersurface far from the black hole the curvature vanishes. Describe the black hole by an Einstein-Rosen bridge (*i.e.*, by two asymptotically flat three-surfaces connected by a throat) and insist that the spacetime be inversion symmetric through the throat. These choices impose the boundary conditions

$$\lim_{r \rightarrow \infty} \psi(r) = 1 \quad \text{asymptotic flatness,} \quad (2.11a)$$

$$\left[ \frac{\partial \psi}{\partial r} + \frac{\psi}{2a} \right]_{r=a} = 0 \quad \text{inversion symmetry,} \quad (2.11b)$$

on  $\psi$  where  $r = a$  is the coordinate location of the throat.

We can now describe how to solve the constraint equations. Let  $K$  vanish on the initial hypersurface; then the Hamiltonian and the momentum constraints (eqs. 2.10) decouple.<sup>†</sup> Pick a conformal background metric  $\bar{\gamma}_{ij}$  (which determines  ${}^{(3)}\bar{\nabla}$ ) and transverse-traceless part  $\bar{A}_{TT}^{ij}$  of the conformal extrinsic curvature. Solve the momentum constraints (eqs. 2.10b) for the longitudinal part of the trace-free conformal extrinsic curvature  $\bar{A}_{ij}$ . Together with  $\bar{A}_{TT}^{ij}$  the trace-free conformal extrinsic curvature is thus fully determined and the Hamiltonian constraint (eq. 2.10a) can be solved for the conformal factor. This determines the three-metric  $\gamma_{ij}$  and its extrinsic curvature  $K^{ij}$  and completes the specification of the initial data.

## C. Three test problems

### 1. Black hole with angular momentum

Focus first on the initial data corresponding to an axisymmetric black hole spacetime with angular momentum. This problem was first examined analytically by [11], and has been explored numerically by [5,6].

Choosing the conformal background metric to be flat (*i.e.*,  $\bar{\gamma}_{ij} = \delta_{ij}$ ), [11] found an analytic solution to the momentum constraints (eqs. 2.10b) that carries angular momentum and obeys the isometry condition at the black hole throat. Draw through any point a sphere centered on

<sup>†</sup>Such a hypersurface is said to have vanishing mean curvature, or be *maximally embedded*.

the black hole throat, and let  $n^i$  be the outward-pointing unit vector to the sphere there. Letting  $J^i$  be the angular momentum of the *physical* space, the Bowen-York solution to the momentum constraints is

$$\bar{A}_{ij} = \frac{3}{r^3} [\epsilon_{aib} J^b n^a n_j + \epsilon_{ajb} J^b n^a n_i]. \quad (2.12)$$

Corresponding to this solution is the Hamiltonian constraint (eq. 2.10a) for the conformal factor  $\psi$ ,

$$\bar{\nabla}^2 \psi + \frac{9}{4} \frac{J^2 \sin^2 \theta}{r^6} \psi^{-7} = 0, \quad (2.13)$$

together with its boundary conditions,

$$\lim_{r \rightarrow \infty} \psi(r) = 1, \quad (2.14a)$$

$$\left[ \frac{\partial \psi}{\partial r} + \frac{1}{2a} \psi \right]_{r=a} = 0, \quad (2.14b)$$

$$\left( \frac{\partial \psi}{\partial \theta} \right)_{\theta=0, \pi} = 0, \quad (2.14c)$$

which result from asymptotic flatness, the isometry condition at the throat (which is located at  $r = a$ ), and axisymmetry respectively. The equation with boundary conditions for the conformal factor is solved on the domain  $a \leq r < \infty$ . Once the conformal factor is determined, the geometry of the initial slice is completely specified.

A useful diagnostic of an initial data slice is to compute the total energy contained in the slice. Ó Murchadha and York [12] have examined the ADM energy (cf. [8]) in terms of the conformal decomposition formalism giving

$$E_{ADM} = \hat{E}_{ADM} - \frac{1}{2\pi} \oint_{\infty} \bar{\nabla}^j \psi d^2 \bar{S}_j, \quad (2.15)$$

where  $\hat{E}_{ADM}$  is the energy of the conformal metric. Thus when the conformal metric is flat, the ADM energy reduces to

$$E_{ADM} = -\frac{1}{2\pi} \oint_{\infty} \bar{\nabla}^j \psi d^2 \bar{S}_j, \quad (2.16)$$

*i.e.*, it is proportional to the integral of the normal component of the gradient of the conformal factor about the sphere at infinity.

## 2. A model problem

Bowen and York [11] also describe a nonlinear “model” of the Hamiltonian constraint equation that can be solved exactly, which we utilize in section V to test our code. The model equation is

$$\bar{\nabla}^2 \psi + \frac{3}{4} \frac{P^2}{r^4} \left( 1 - \frac{a^2}{r^2} \right)^2 \psi^{-7} = 0, \quad (2.17)$$

with  $P$  a constant. Together with the boundary conditions described above (eqs. 2.14), equation 2.17 has the solution

$$\psi = \left[ 1 + \frac{2E}{r} + 6 \frac{a^2}{r^2} + \frac{2a^2 E}{r^3} + \frac{a^4}{r^4} \right]^{1/4}, \quad (2.18a)$$

where

$$E = (P^2 + 4a^2)^{1/2}. \quad (2.18b)$$

If we evaluate equation 2.16 for this solution, we find that it has ADM energy  $E$ .

## 3. Black hole plus Brill wave

The second physical problem upon which we demonstrate the use of spectral methods for numerical relativity is that of a black hole superposed with a Brill [13] wave, a problem studied using FD by [7].

Following [7], let the initial slice be a spacetime isometry surface (*i.e.*, time symmetric); then, the extrinsic curvature  $K_{ij}$  vanishes and the momentum constraints (eqs. 2.10b) are trivially satisfied.

To determine the conformal factor the Hamiltonian constraint (eq. 2.10a) must be solved, which requires the specification of a conformal background metric. Let the line-element of the conformal background metric have the form

$$d\bar{s}^2 = [e^{2q} (dr^2 + r^2 d\theta^2) + r^2 \sin^2 \theta d\phi^2], \quad (2.19)$$

where

$$q := A \sin^n \theta \left\{ \exp \left[ - \left( \frac{\eta + \eta_0}{\sigma} \right)^2 \right] + \exp \left[ - \left( \frac{\eta - \eta_0}{\sigma} \right)^2 \right] \right\}, \quad (2.20a)$$

$$\eta := \ln \frac{r}{a}, \quad (2.20b)$$

$n$  is an even integer, and  $A$ ,  $\eta_0$ , and  $\sigma$  are constant parameters that describe the superposed Brill wave’s amplitude, position, and width, respectively. With this choice the Hamiltonian constraint equation becomes

$$\begin{aligned} \frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r} \frac{\partial \psi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial \theta^2} + \frac{\cot \theta}{r^2} \frac{\partial \psi}{\partial \theta} \\ + \frac{\psi}{4} \left( \frac{\partial^2 q}{\partial r^2} + \frac{1}{r} \frac{\partial q}{\partial r} + \frac{1}{r^2} \frac{\partial^2 q}{\partial \theta^2} \right) = 0. \end{aligned} \quad (2.21)$$

The boundary conditions of asymptotic flatness and inversion symmetry are again given by equations 2.14. Furthermore, since the conformal metric  $\bar{\gamma}_{ij}$  has no “ $1/r$ ” parts in its expansion at infinity, its energy vanishes and the ADM energy for these slices is given by equation 2.16.

### III. SPECTRAL METHODS

#### A. Introduction

Consider an elliptic differential equation, specified by the operator  $L$  on the  $d$ -dimensional open, simply-connected domain  $\mathcal{D}$ , with boundary conditions given by the operator  $S$  on the boundary  $\partial\mathcal{D}$ :

$$L(u)(\mathbf{x}) = f(\mathbf{x}) \quad \mathbf{x} \in \mathcal{D}, \quad (3.1a)$$

$$S(u)(\mathbf{x}) = g(\mathbf{x}) \quad \mathbf{x} \in \partial\mathcal{D}. \quad (3.1b)$$

There may be more than one boundary condition, in which case we can index  $S$  and  $g$  over the boundary conditions.

Approximate the solution  $u(\mathbf{x})$  to this system as a sum over a sequence of *basis functions*  $\phi_k(\mathbf{x})$  on  $\mathcal{D} + \partial\mathcal{D}$ ,

$$u_N(\mathbf{x}) = \sum_{k=0}^{N-1} \tilde{u}_k \phi_k(\mathbf{x}), \quad (3.2)$$

where the  $\tilde{u}_k$  are constant coefficients. Corresponding to the approximate solution  $u_N$  is a residual  $R_N$  on  $\mathcal{D}$  and  $r_N$  on  $\partial\mathcal{D}$ :

$$R_N = L(u_N) - f \quad \text{on } \mathcal{D}, \quad (3.3a)$$

$$r_N = S(u_N) - g \quad \text{on } \partial\mathcal{D}. \quad (3.3b)$$

The residual vanishes everywhere for the exact solution  $u$ .

In PSC we determine the coefficients  $\tilde{u}_k$  by requiring that  $u_N$  satisfies the differential equation and boundary conditions *exactly* at a fixed set of *collocation points*  $x_n$ : *i.e.*, we require that

$$0 = L[u_N(x_n)] - f(x_n) \quad \text{for } x_n \text{ in } \mathcal{D}, \quad (3.4a)$$

$$0 = S[u_N(x_n)] - g(x_n) \quad \text{for } x_n \text{ on } \partial\mathcal{D}, \quad (3.4b)$$

for all  $n$ . When the expansion functions and collocation points are chosen appropriately a numerical solution of these equations can be found very efficiently. In the following subsection we discuss choices of the expansion basis and collocation points.

#### B. Expansion basis and collocation points

In PSC we require that the approximate solution  $u_N$  satisfies the differential equation and boundary conditions exactly at the  $N$  collocation points  $x_n$ . The basis  $\phi_k$  should not constrain the values of the approximation at the collocation points; correspondingly, we can write the basis as a set of  $N$  functions  $\phi_k(x)$  that satisfy a discrete orthogonality relationship on the collocation points  $x_n$ :

$$\sum_{n=0}^{N-1} \phi_j(x_n) \phi_k^*(x_n) = \nu_k^2 \delta_{jk}, \quad (3.5)$$

where the  $\nu_k$  are normalization constants. Note that the basis functions are inextricably linked with the collocation points.

It is sometimes the case that the basis can be chosen so that the boundary conditions are automatically satisfied. For example, consider a one-dimensional problem on the interval

$$\mathbb{I} = [-1, 1]. \quad (3.6)$$

If the boundary conditions are periodic then each element of the basis

$$\phi_k(x) = \exp[\pi i (x+1)k], \quad (3.7a)$$

satisfies the boundary conditions; correspondingly, the approximate solution  $u_N$  automatically satisfies the boundary conditions. If, in addition, we choose the collocation points

$$x_n = \frac{2n}{N} - 1, \quad (3.7b)$$

then the basis satisfies the discrete orthogonality relation

$$\delta_{jk} = \frac{1}{N} \sum_{n=0}^{N-1} \phi_j(x_n) \phi_k^*(x_n). \quad (3.7c)$$

In an arbitrary basis, or with arbitrarily chosen collocation points, finding the  $\tilde{u}_k$  from the  $u_N(x_n)$  requires the solution of a general linear system of  $N$  equations in  $N$  unknowns, which involves  $\mathcal{O}(N^3)$  operations. For the basis and collocation points given in equations 3.7 the  $\tilde{u}_k$  can be determined from the  $u_N(x_n)$  quickly and efficiently via the Fast Fourier Transform in  $\mathcal{O}(N \ln N)$  operations.

Arbitrary derivatives of the  $u_N$  can also be computed quickly: writing

$$\frac{d^p u_N}{dx^p} = \sum_{k=0}^{N-1} \tilde{u}_k^{(p)} \phi_k(x), \quad (3.8a)$$

we see immediately that

$$\tilde{u}_k^{(p)} = (\pi i k)^p. \quad (3.8b)$$

Consequently, any derivative of  $u_N$  can be evaluated at all the collocation points in just  $\mathcal{O}(N \ln N)$  operations.

The ability to evaluate efficiently the derivatives of  $u_N$  at the collocation points is much more important than finding a basis whose individual members satisfy the boundary conditions. In the case of periodic boundary conditions we can have our cake and eat it, too. More generally we choose a basis in which we can efficiently compute the derivatives of  $u_N$  at the collocation points and require separately that the approximate solution  $u_N$  satisfy the boundary conditions at collocation points on the boundary.

For general boundary conditions a basis of Chebyshev polynomials often meets all of our requirements.<sup>‡</sup> Recall that the Chebyshev polynomials are defined on  $\mathbb{I}$  by

$$T_k(x) = \cos(k \cos^{-1} x). \quad (3.9)$$

A simple recursion relation allows us to find the derivative of  $u_N$  as another sum over Chebyshev polynomials: if <sup>§</sup>

$$u_N(x) = \sum_{k=0}^N \tilde{u}_k T_k(x), \quad (3.10)$$

then

$$\frac{du_N}{dx}(x) = \sum_{k=0}^{N-1} \tilde{u}'_k T_k(x), \quad (3.11)$$

where

$$c_k \tilde{u}'_k = \tilde{u}'_{k+2} + 2(k+1)\tilde{u}_{k+1}, \quad (3.12)$$

with

$$c_k = \begin{cases} 2 & k=0 \\ 1 & k \geq 1. \end{cases} \quad (3.13)$$

If we choose collocation points  $x_n$  (for  $0 \leq n \leq N$ ) according to

$$x_n = \cos \frac{\pi n}{N}, \quad (3.14)$$

then the Chebyshev polynomials satisfy the discrete orthogonality relation

$$\delta_{jk} = \frac{2}{N\bar{c}_k} \sum_{n=0}^N \frac{1}{\bar{c}_n} T_j(x_n) T_k(x_n), \quad (3.15)$$

where

$$\bar{c}_k = \begin{cases} 2 & k=0 \text{ or } N \\ 1 & \text{otherwise.} \end{cases} \quad (3.16)$$

Finally, exploiting the relation between the Chebyshev polynomials and the Fourier basis (cf. 3.9) allows us to find the  $\tilde{u}_k$  from the  $u_N(x_n)$  in  $\mathcal{O}(N \ln N)$  time using a

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<sup>‡</sup>The geometry of a problem might suggest other expansion functions, such as Legendre polynomials; however, a Chebyshev expansion does quite well and has the added convenience that, with appropriately chosen collocation points, only  $\mathcal{O}(N \ln N)$  are required to convert from the expansion coefficients to the function values at the collocation points and vice versa [14].

<sup>§</sup>For Chebyshev bases the conventional notation is that  $k$  runs from 0 to  $N$ , not  $N-1$ ; thus, there are  $N+1$  coefficients and collocation points.

fast transform [2, appendix B]. With an expansion basis of Chebyshev polynomials and an appropriate choice of collocation points we can thus evaluate derivatives of arbitrary order at the collocation points in  $\mathcal{O}(N \ln N)$  operations.

For problems on an arbitrary domain of dimension  $d$  greater than unity it is rarely the case that we can find a basis which permits rapid evaluation of derivatives. If the domain can be mapped smoothly to  $\mathbb{I}^d$  then we can write

$$u_{N^{(1)} \dots N^{(d)}}(\mathbf{x}) = \sum_{k_1=0}^{N^{(1)}} \dots \sum_{k_d=0}^{N^{(d)}} \tilde{u}_{k_1 \dots k_d} \phi_{k_1 \dots k_d}(\mathbf{x}), \quad (3.17a)$$

where

$$\phi_{k_1 \dots k_d}(\mathbf{x}) = \prod_{\ell=1}^d \phi_{k_\ell}^{(\ell)}(x^{(\ell)}), \quad (3.17b)$$

$$\mathbf{x} = (x^{(1)}, \dots, x^{(d)}), \quad (3.17c)$$

and the  $\phi_k^{(\ell)}$ , for fixed  $\ell$ , is a basis on  $\mathbb{I}$  which permits fast evaluation of derivatives with respect to its argument (*e.g.*, Chebyshev polynomials). Associated with each set of basis functions are the collocation points  $x_n^{(\ell)}$ ; correspondingly, the collocation points associated with  $\phi_{k_1 \dots k_d}$  are just the  $N_1 \dots N_d$ -tuples

$$\mathbf{x}_{n_1 \dots n_d} = (x_{n_1}^{(1)}, \dots, x_{n_d}^{(d)}). \quad (3.17d)$$

With this choice of basis and collocation points we can evaluate efficiently arbitrary derivatives of an approximation  $u_{N^{(1)} \dots N^{(d)}}$ . If the domain cannot be mapped smoothly to a  $d$ -cube in  $\mathbb{R}^d$ , either more sophisticated methods such as domain decomposition [1,2] must be used, or the problem may not be amenable to solution by PSC.

### C. Solving the system of equations

The expansion basis, collocation points and differential equation with boundary conditions determine a system of equations for the coefficients  $\tilde{u}_k$  or, equivalently, the approximate solution  $u_N$  evaluated at the collocation points. Iterative solution methods (which require as few as  $\mathcal{O}(N \ln N)$  operations) work well to solve the kind of systems of equations that arise from the application of a PSC method.

If the elliptic system being solved is linear then the algebraic equations arising from either a FD or a PSC method are also linear and a unique solution is guaranteed. If, on the other hand, the differential system is nonlinear, then the equations arising from FD or PSC are also nonlinear and a unique solution is not guaranteed. Newton's method [1, sec. 12.13 and appendices C

and D], where one solves the linearized equations beginning with a guess and then iterating, works well for these types of equations. As long as a good initial guess is chosen, the iteration will usually converge. In appendix A we describe in detail the variant of Newton's method (Richardson's iteration) that we have used to solve the nonlinear system of algebraic equations that arise when we apply PSC to solve the Hamiltonian constraint equations as posed in section II.

#### IV. COMPARING FINITE DIFFERENCE AND PSEUDOSPECTRAL COLLOCATION METHODS

##### A. Introduction

Finite differencing and pseudospectral collocation are alternative ways to find approximate solutions to a system of differential equations. Consider the Poisson problem in one dimension:

$$\frac{d^2 u}{dx^2} = f(x), \quad (4.1a)$$

on the interval  $\mathbb{I}$  with Dirichlet boundary conditions

$$u(-1) = u(1) = 0. \quad (4.1b)$$

In a FD approach to this problem we seek the values of  $u$  at discrete points  $x_n$ , say

$$x_n = -1 + \frac{2n}{N}, \quad (4.2)$$

for  $n = 0, 1, \dots, N$ . Algebraic equations are found by approximating the differential operator  $d^2 u/dx^2$  in equation 4.1a by a ratio of differences: *e.g.*,

$$\frac{d^2 u}{dx^2}(x_n) \simeq \frac{u_{n+1} - 2u_n + u_{n-1}}{\Delta x^2}, \quad (4.3)$$

for integer  $n = 1, 2, \dots, N-1$  where

$$u_n := u(x_n), \quad (4.4a)$$

$$\Delta x := 2/N. \quad (4.4b)$$

With this discretization the differential equation 4.1a yields  $N-1$  equations for the  $N+1$  unknown  $u_n$ . The boundary conditions (eq. 4.1b) yield two more equations, completely determining the  $u_n$ :

$$\frac{u_{n+1} - 2u_n + u_{n-1}}{\Delta x^2} = f(x_n) \quad \text{for } n = 1, 2, \dots, N-1, \quad (4.5a)$$

$$u_0 = 0, \quad (4.5b)$$

$$u_N = 0. \quad (4.5c)$$

The solution to these equations is the FD approximation to  $u(x)$  at the points  $x_n$ .

The FD solution to equations 4.1 begins by approximating the differential equations. In the PSC method, on the other hand, we first approximate the solution at all points in  $\mathbb{I}$  by a sum over a finite set of basis functions. For this example, we choose a Chebyshev basis; so, we write

$$u_N(x) = \sum_{k=0}^N \tilde{u}_k T_k(x). \quad (4.6)$$

Now insist that  $u_N$  satisfies the differential equation and boundary conditions exactly at the collocation points

$$x_n = \cos \frac{\pi n}{N}, \quad (4.7)$$

for  $n = 0, 1, \dots, N$ . In particular, we require that the boundary conditions are satisfied and that, in addition, the differential equation is satisfied for integer  $n$  ranging from 1 to  $N-1$ :

$$u_N(x_0) = 0, \quad (4.8a)$$

$$u_N(x_N) = 0, \quad (4.8b)$$

$$\frac{d^2 u_N}{dx^2}(x_n) = f(x_n). \quad (4.8c)$$

To evaluate equation 4.8c note that  $d^2 u_N/dx^2$  can be written as

$$\frac{d^2 u_N}{dx^2}(x_n) = \sum_{m=0}^N d_{nm}^{(2)} u_N(x_m). \quad (4.9a)$$

The  $d_{nm}^{(2)}$  can be determined by noting that

$$\frac{d^2 u_N}{dx^2}(x_n) = \sum_{k=0}^N \tilde{u}_k'' T_k(x_n), \quad (4.9b)$$

with

$$\begin{aligned} c_k \tilde{u}_k'' &= \tilde{u}_{k+2}'' + 2(k+1) \tilde{u}_{k+1}', \\ c_k \tilde{u}_k' &= \tilde{u}_{k+2}' + 2(k+1) \tilde{u}_{k+1}, \end{aligned} \quad (4.9c)$$

and

$$\tilde{u}_k = \frac{2}{N \bar{c}_k} \sum_{n=0}^N \frac{1}{\bar{c}_n} u_N(x_n) T_k(x_n), \quad (4.9d)$$

where  $c_k$  and  $\bar{c}_k$  are given by equations 3.13 and 3.16, respectively.

The result is, again, a set of algebraic equations for  $u_N(x_n)$ : the values of the approximate solution at the collocation points. Finding the  $u_N(x_n)$  yields an approximate solution to the differential equation over the entire domain  $\mathbb{I}$  since the spectral coefficients  $\tilde{u}_k$  are given by equation 4.9d.\*\*

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\*\* Alternatively, we could have constructed a system of equations in terms of the unknown spectral coefficients. This would correspond to a spectral tau method: *cf.* [1,2].

For the linear problem posed here the solution to the algebraic system of equations that arise in either a FD or PSC solution can be solved directly or by any of the many standard iterative methods. For nonlinear problems the systems are generally solved by linearizing the equations about an initial guess and then iterating the solution until it converges. We discuss one method of solution in appendix A.

## B. Convergence of approximations

In either a FD or PSC solution to a differential equation with boundary conditions we expect that, as  $N$  tends to infinity, the approximate solution should become arbitrarily accurate. For large  $N$ , the  $L_2$  error in a FD approximation converges upon the exact solution as  $N^{-p}$  for positive integer  $p$ . The value of  $p$  depends on the smoothness of  $f$  and the error in the approximation of the differential operator (in the example above,  $d^2/dx^2$ ). Assuming that  $f$  is smooth the rate of convergence (measured by the  $L_2$  error of the FD solution) is  $N^{-p}$  when the truncation error of the differential operator is  $\mathcal{O}(\Delta x^p)$ .

In contrast, when the solution  $u$  is smooth the error made by a properly formulated spectral approximation decreases faster than any fixed power of  $N$  (where  $N$  is now the number of collocation points or basis functions).<sup>††</sup> For a heuristic understanding of this rapid convergence, note first that a PSC solution's derivatives at each collocation point involve all the  $\{u_N(x_n)\}$  (cf. eq. 4.9). Correspondingly, it is as exact as possible, given the information available at the  $N$  collocation points. This suggests that an order  $N$  collocation spectral approximation to the derivatives of the unknown should make errors on order  $\mathcal{O}(\Delta x^N)$ . The interval  $\Delta x$ , however, is also proportional to  $N^{-1}$ ; so, we expect that the error in the spectral solution  $u_N$  should vary as  $\mathcal{O}(N^{-N})$ . A more rigorous analysis using convergence theory [1, chapter 2] shows that for any function which is analytic on the domain of interest, a Chebyshev expansion will converge exponentially (*i.e.* as  $\mathcal{O}(e^{-N})$ ). If the function is also periodic then a Fourier expansion will converge exponentially.

## C. Computational cost of solutions

The computational cost, in time, of a FD solution to a system of elliptic differential equations scales linearly with the number of grid points  $N$  while the accuracy  $\epsilon$  of the solution scales as  $N^{-p}$ , where  $p$  is the order of the

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<sup>††</sup>In addition the individual spectral coefficient  $\tilde{u}_k$  should decrease exponentially with  $N$  once the problem is sufficiently resolved.

FD operator truncation error. Correspondingly, the cost  $K_{\text{FD}}$  for a given accuracy scales as

$$K_{\text{FD}} \sim \epsilon^{-1/p}. \quad (4.10a)$$

The cost  $K_{\text{PSC}}$  of a PSC solution to the same system, on the other hand, scales as  $N \ln N$  (for an iterative solution) while  $\epsilon$  scales as  $\exp(-N)$ ; consequently, the cost scales with accuracy  $\epsilon$  as

$$K_{\text{PSC}} \sim -(\ln \epsilon) \ln(-\ln \epsilon). \quad (4.10b)$$

Since it is the computational cost required to achieve a given accuracy that is important, the more rapid convergence of a PSC solution confers upon it a clear advantage. This advantage is made clear by considering how the ratio of costs scales with accuracy:

$$\frac{K_{\text{PSC}}}{K_{\text{FD}}} \sim -\epsilon^{1/p} \ln \epsilon \ln(-\ln \epsilon), \quad (4.11)$$

which tends to zero with  $\epsilon$ ; consequently, increasing accuracy with a PSC solution is always more efficient than with a FD solution.

The equations that arise from either a FD or PSC treatment of an elliptic differential system are typically solved using iterative methods; thus, *at fixed resolution* the storage requirements for either solution method are equivalent. As we have seen, however, fixed resolution does not correspond to fixed solution accuracy. As the desired solution accuracy increases the storage requirements of a PSC solution fall relative to those of an FD solution a factor of  $-\epsilon^{1/p} \ln \epsilon$ .

## V. SOLVING THE HAMILTONIAN CONSTRAINT

### A. Nonlinear model problem

As a first example we solve the model Hamiltonian constraint equation described in section II C 2, equation 2.17:

$$\bar{\nabla}^2 \psi + \frac{3}{4} \frac{P^2}{r^4} \left(1 - \frac{a^2}{r^2}\right)^2 \psi^{-7} = 0, \quad (5.1a)$$

for  $r \in [a, \infty)$  with  $P$  a constant and with the boundary conditions

$$\lim_{r \rightarrow \infty} \psi(r) = 1 \quad \text{asymptotic flatness}, \quad (5.1b)$$

$$\left[ \frac{\partial \psi}{\partial r} + \frac{1}{2a} \psi \right]_{r=a} = 0 \quad \text{inversion symmetry}, \quad (5.1c)$$

$$\left( \frac{\partial \psi}{\partial \theta} \right)_{\theta=0, \pi} = 0 \quad \text{axisymmetry}. \quad (5.1d)$$

For this model problem the solution  $\psi$  is



$$\psi = \left[ 1 + \frac{2E}{r} + 6\frac{a^2}{r^2} + \frac{2a^2E}{r^3} + \frac{a^4}{r^4} \right]^{1/4}, \quad (5.2a)$$

where

$$E = (P^2 + 4a^2)^{1/2}, \quad (5.2b)$$

is also the ADM energy for the initial data (cf. eq. 2.16).

As described this problem is spherically symmetric; nevertheless, we treat it as axisymmetric to illustrate the methods used to solve the Hamiltonian constraint for the black hole with angular momentum (cf. sec. II C 1) and the black hole plus Brill wave problems (cf. sec. II C 3).

As a first step we map the domain  $r \in [a, \infty)$ ,  $\theta \in [0, \pi]$  to a square in  $\mathbb{R}^2$ : letting

$$x = \frac{2a}{r} - 1, \quad (5.3a)$$

$$y = \cos \theta, \quad (5.3b)$$

we have  $x \in (-1, 1]$  and  $y \in [-1, 1]$ . In terms of the  $(x, y)$  coordinates, the model Hamiltonian constraint (eq. 5.1a) becomes

$$(x+1)^2 \frac{\partial^2 \psi}{\partial x^2} + (1-y^2) \frac{\partial^2 \psi}{\partial y^2} - 2y \frac{\partial \psi}{\partial y} + \frac{3}{256} \left( \frac{P}{a} \right)^2 (x+1)^2 (3-2x-x^2)^2 \psi^{-7} = 0, \quad (5.4)$$

subject to the boundary conditions

$$\lim_{x \rightarrow -1} \psi = 1, \quad (5.5a)$$

$$\left[ \frac{\partial \psi}{\partial x} - \frac{1}{4} \psi \right]_{x=1} = 0. \quad (5.5b)$$

Note that with our choice of variables and expansion bases the angular boundary conditions (eq. 5.1d) are automatically satisfied.

Since  $\psi$  is not periodic in either  $x$  or  $y$ , we adopt a Chebyshev basis for the approximate solution:

$$\psi_{N_x, N_y}(x, y) = \sum_{j=0}^{N_x} \sum_{k=0}^{N_y} \tilde{\psi}_{jk} T_j(x) T_k(y), \quad (5.6a)$$

with the corresponding collocation points

$$x_j = \cos \frac{\pi j}{N_x}, \quad (5.6b)$$

$$y_k = \cos \frac{\pi k}{N_y}. \quad (5.6c)$$

For this problem, focus on approximations

$$\Psi_\ell = \psi_{4\ell, 4}, \quad (5.7)$$

for integer  $\ell$ . We keep  $N_y$  fixed as the model problem is independent of  $y$ .

Following the discussion in appendix A, solve the PSC equations using Richardson's iteration with a second-order FD preconditioner. To obtain  $\Psi_\ell$ , we need an initial guess  $\Psi_\ell^{(0)}$  to begin the iteration. For the lowest resolution expansion ( $N_x = 4$ ) begin the iteration with the guess

$$\Psi_1^{(0)}(x, y) = \frac{(3+x)}{2}, \quad (5.8)$$

which is the trivial solution for  $P = 0$ . Applying Richardson's iteration will then give us the approximate solution  $\Psi_1$ . Through the expansion 5.6a this determines an approximation for  $\psi$  everywhere; in particular, it determines an approximation at the collocation points corresponding to  $N_x = 8$ , which we then use as the initial guess for determining the approximate solution  $\Psi_2$ . In this same way we use a lower-resolution approximate solution as the initial guess for the approximate solution at the next higher-resolution, *i.e.*

$$\Psi_\ell^{(0)} = \Psi_{\ell-1}. \quad (5.9)$$

To investigate the accuracy of our solution as a function of resolution (basis dimension for PSC, number of grid points for FD) we evaluate a number of solutions differing only in resolution and evaluate several different error measures.

1. For this problem we know the exact solution (cf. 5.2); so, we calculate the  $L_2$  norm of the absolute error as a function of  $\ell$ :

$$\begin{aligned} \Delta \Psi_\ell &= \left\{ \sum_{j=0}^{N_x} \sum_{k=0}^{N_y} \frac{1}{N_x N_y \bar{c}_j \bar{c}_k} [\Psi_\ell(x_j, x_k) - \psi(x_j, x_k)]^2 \right\}^{1/2} \\ &:= \|\Psi_\ell - \psi\|_2, \end{aligned} \quad (5.10)$$

where  $c_k$  is given by equation 3.16.

2. We can also characterize the convergence of the approximate solutions  $\Psi_\ell$  by calculating the  $L_2$  norm of the difference between the successive approximate solutions:

$$\delta \Psi_\ell = \|\Psi_\ell - \Psi_{\ell-1}\|_2. \quad (5.11)$$

The errors  $\delta \Psi$  and  $\Delta \Psi$  are defined for either FD or PSC solutions.

3. We also evaluate, by analogy with  $\Delta \Psi$  and  $\delta \Psi$ , the quantities

$$\Delta E_\ell = |E_\ell - E|, \quad (5.12)$$

$$\delta E_\ell = |E_\ell - E_{\ell-1}|, \quad (5.13)$$

where  $E_\ell$  is the ADM mass-energy associated with the approximate conformal factor  $\Psi_\ell$ . We evaluate  $E$  using equation 2.16.

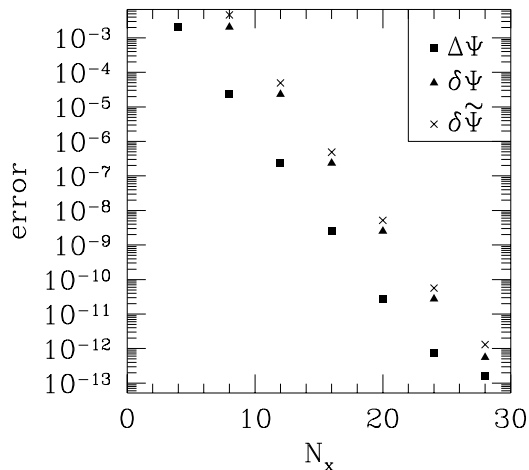


FIG. 1. Spectral convergence for a nonlinear model problem. Plotted are a measure of the absolute error  $\Delta\Psi_\ell$ , and two approximate measures of the error  $\delta\Psi_\ell$  and  $\delta\tilde{\Psi}_\ell$  as a function of  $N_x$ , the number of radial functions, for the case  $P = 1$ .

4. For PSC solutions only we define the relative error measure

$$\delta\tilde{\Psi}_\ell = \sum_{j=0}^{N_x} \sum_{k=0}^{N_y} \left| \tilde{\psi}_{jk}^{(\ell)} - \tilde{\psi}_{jk}^{(\ell-1)} \right|, \quad (5.14)$$

which characterizes the changes in the spectral coefficients as the order of the approximation increases.

For a properly formulated spectral method, all of our error measures should decrease exponentially with  $N$  if the solution to the problem is analytic.

Figure 1 shows the absolute and relative errors  $\Delta\Psi_\ell$  and  $\delta\Psi_\ell$ , along with the change in the spectral coefficients  $\delta\tilde{\Psi}_\ell$ , for  $P = 1$ . The exponential convergence of the solution with increasing  $N_x$  is apparent. Experience shows that as the problem becomes more nonlinear (*i.e.*,  $P$  becomes larger) more terms are needed in the expansion in order to achieve the same accuracy.

This system of equations has also been solved using FD methods [6]. A point comparison is telling: in [6] a second order accurate FD solution with a resolution of 1024 radial points were required for a solution with a  $\Delta E \simeq 10^{-5}$ , independent of  $P$ . The PSC solution described here achieves the same accuracy using an expansion with only 12 radial functions for  $P = 1$ , and 24 functions for  $P = 10$ . In either case a PSC solution

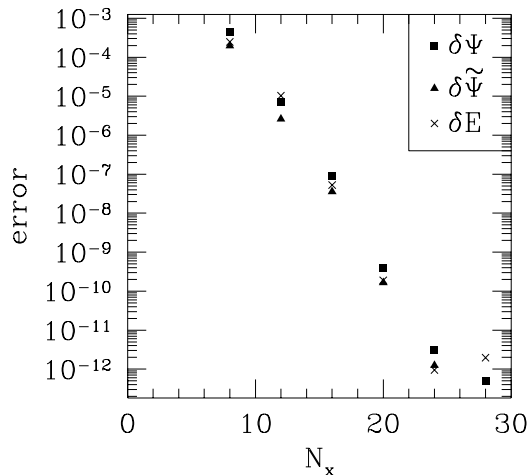


FIG. 2. Spectral convergence for the solution of the Hamiltonian constraint equation for a black hole with angular momentum. Plotted are three approximate measures of the error  $\delta\Psi_\ell$ ,  $\delta\tilde{\Psi}_\ell$  and  $\delta E$  as a function of  $N_x$ , the number of radial functions, for  $J = 1$ .

with an accuracy of  $\Delta E \approx 10^{-10}$  is obtained by doubling the number of radial functions. To achieve the same accuracy the FD approximation would require (assuming second order FD) a resolution of  $3 \times 10^5$  radial points.

## B. Black hole with angular momentum

Now turn to consider a truly non-radial, but still axisymmetric, problem: a rotating black hole (cf. II C 1). As before (cf. 5.3) we map the semi-infinite domain  $r \geq a$  to the finite box  $x \in (-1, 1]$ ,  $y \in [-1, 1]$ , obtaining the system of equations

$$(x+1)^2 \frac{\partial^2 \psi}{\partial x^2} + (1-y^2) \frac{\partial^2 \psi}{\partial y^2} - 2y \frac{\partial \psi}{\partial y} + \frac{9}{64} \left( \frac{J}{a^2} \right)^2 (x+1)^4 (1-y^2) \psi^{-7} = 0, \quad (5.15)$$

subject to the boundary conditions given in equations 5.5.

For this problem we do not have the exact solution; so, we consider only the relative errors  $\delta\Psi$ ,  $\delta\tilde{\Psi}$  and  $\delta E$ . Figure 2 (3) shows these quantities as functions of  $N_x$  for  $J/M^2$  equal to 1 (100). For these solutions  $\Psi_\ell = \psi_{4\ell, N_y}$ ,

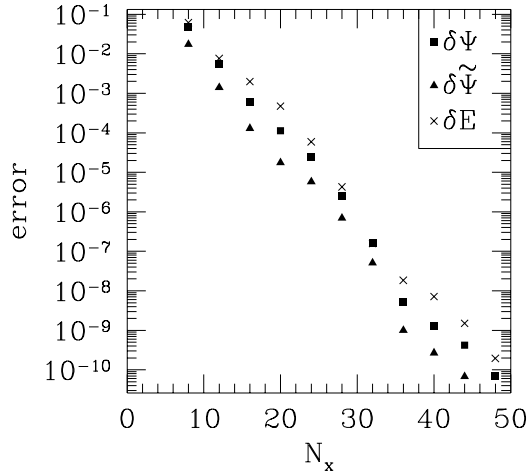


FIG. 3. Same as figure 2 with  $J = 100$ .

where initially  $N_y = 4$  and is incremented by two<sup>††</sup> whenever the difference between  $\delta\Psi_\ell$  with and without the increment was greater than ten percent. Again we see rapid, exponential convergence of the solution with  $N$ .

This problem has also been solved using second order FD [6]. For a solution accuracy  $\delta E \simeq 10^{-5}$ , [6] found that a resolution 1024 radial and 384 angular grid points was required, roughly independent of the value of  $J$ . We find that PSC achieves the same accuracy with an expansion basis of 12 radial (and 4 angular) functions for  $J = 1$ , and 24 radial (and 8 angular) functions for  $J = 100$ . Solution accuracies of  $10^{-10}$  can be obtained for the PSC solution simply by doubling the size of the expansion basis (in  $x$  and  $y$ ). For a similar increase in accuracy of the FD solution a grid approximately 300 times larger in each dimension would be required.

### C. Black hole plus Brill wave

As a final example we consider the Hamiltonian constraint for a black hole superposed with a Brill wave. After mapping this problem to the  $(x, y)$  domain we obtain

<sup>††</sup>Along with axisymmetry, this problem has equatorial plane symmetry so  $\Psi_\ell$  is even in  $y$ . By exploiting this symmetry, we could reduce our number of angular functions by a factor of two

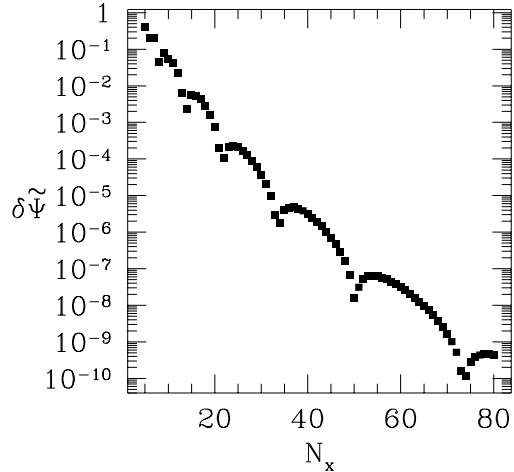


FIG. 4. Spectral convergence for the solution of the Hamiltonian constraint equation for a black hole plus Brill wave. Plotted is an approximate measure of the error  $\delta\tilde{\Psi}_\ell$  as a function of  $N_x$ , the number of radial functions, for the case  $A = \eta_0 = \sigma = 1$ ,  $n = 2$ .

the system of equations

$$(x+1)^2 \frac{\partial^2 \Psi}{\partial x^2} + (1-y^2) \frac{\partial^2 \Psi}{\partial y^2} - 2y \frac{\partial \Psi}{\partial y} + \frac{\Psi R}{4} = 0, \quad (5.16a)$$

with

$$R = (x+1)^2 \frac{\partial^2 q}{\partial x^2} + (x+1) \frac{\partial q}{\partial x} + (1-y^2) \frac{\partial^2 q}{\partial y^2} - y \frac{\partial q}{\partial y}, \quad (5.16b)$$

where  $q$  is given by equation 2.20a, and subject to the boundary conditions 5.5.

In figure 4 we show  $\delta\tilde{\Psi}$  as a function of  $N_x$  for the Brill wave parameters  $\sigma = A = \eta_0 = 1$  and  $n = 2$ . For these solutions  $\Psi_\ell = \psi_{4\ell, N_y}$  where initially  $N_y = 4$ , and is incremented by two whenever the difference between  $\delta\Psi_\ell$  with and without the increment was greater than ten percent. The convergence, while rapid, is not quite exponential. In addition, the nearly exponentially decreasing error is impressed with a wave that is nearly periodic in spectral resolution  $\log N_x$ . We attribute this behavior to the resolution of the factor  $R$  (cf. eq. 5.16b and also eq. 2.20a for  $q$ ). Figure 5 shows the error  $\Delta R$  obtained when we form approximate  $R_{N_x, N_y}$  according to

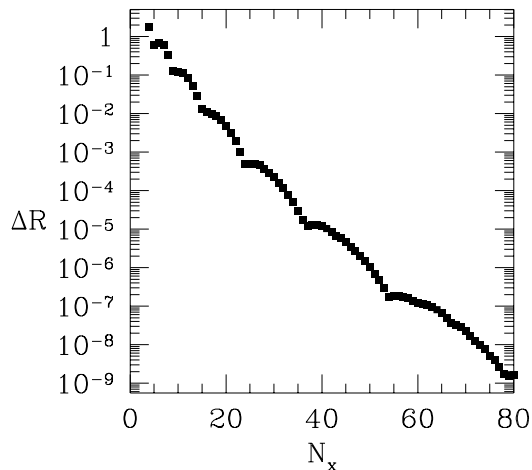


FIG. 5. The error in the spectral representation of  $R$  (equation 5.16b) for the case shown in figure 4

$$R_{N_x, N_y} = \sum_{j=0}^{N_x} \sum_{k=0}^{N_y} \tilde{R}_{jk} T_j(x) T_k(y), \quad (5.17a)$$

with

$$\tilde{R}_{jk} = \frac{4}{N_x N_y \bar{c}_k \bar{c}_j} \sum_{\ell=0}^{N_x} \sum_{m=0}^{N_y} \frac{1}{\bar{c}_\ell \bar{c}_m} T_j(x_\ell) T_k(y_m) R(x_\ell, y_m). \quad (5.17b)$$

The structure in the solution is the same as the structure in the Chebyshev approximation to  $R$ .

This problem has also been solved using FD methods [7], enabling us to compare the resolution required for approximate FD or PSC solution for a given accuracy. With second order FD a solution whose error  $\delta E$  is  $3 \times 10^{-5}$  required a resolution of 400 radial and 105 angular grid points. To achieve the same accuracy the PSC solution described here requires a basis of only 36 radial (and 12 angular) Chebyshev polynomials.

## VI. DISCUSSION

Pseudospectral collocation is a very efficient way of solving the nonlinear elliptic equations that arise in numerical relativity. These problems typically have smooth solutions; correspondingly, the approximate solutions obtained using pseudospectral collocation converge upon

the exact solution exponentially with the number of collocation points. As a result, the cost of a high accuracy pseudospectral solution is not significantly greater than the cost of a similar solution of moderate accuracy. Since the computational burden of solving the pseudospectral collocation equations with a given number of collocation points is no greater than that required to solve the finite difference equations for the same number of grid points, the computational demands of a pseudospectral collocation solution are far less than those of a finite difference solution for even modest accuracy.

Another important advantage of a pseudospectral collocation solution over a finite differencing solution involves the formulation of the boundary conditions. In a finite difference solution the boundary conditions must be reformulated as finite difference equations or incorporated approximately into the formulation of the finite difference operator of the differential equations being solved. This generally involves the introduction of auxiliary boundary conditions, which are not part of the original problem. For example, consider the second order elliptic equation on  $\mathbb{I}$ :

$$\frac{d^2 u}{dx^2} = f(x), \quad (6.1a)$$

$$u(-1) = u(1) = 0. \quad (6.1b)$$

A fourth-order accurate finite difference approximation to the differential operator  $d^2/dx^2$  is

$$\frac{16(u_{j-1} - 2u_j + u_{j+1}) - (u_{j-2} - 2u_j + u_{j+2})}{\Delta x^2} = f(x_j), \quad (6.2)$$

where

$$u_j = u(j\Delta x). \quad (6.3)$$

Before this finite difference operator can be used in equation 6.1 it must be modified at the grid points  $-1 + \Delta x$  and  $1 - \Delta x$  since  $-1 - \Delta x$  and  $1 + \Delta x$  both lie outside the computational domain. In this case, four boundary conditions are required (at  $x$  equal to  $-1$ ,  $-1 + \Delta x$ ,  $1 - \Delta x$  and  $1$ ) even though the second order equation 6.1a properly admits of only two boundary conditions.

In pseudospectral collocation, on the other hand, no auxiliary boundary conditions need be formulated: the approximate solution is expressed as an analytic function, which is required to satisfy the boundary condition equations exactly at the collocation points on the boundary.

These advantages of pseudospectral collocation solution come at a cost. When properly implemented the computational expense of pseudospectral collocation may be considerably less than the expense of finite differencing; however, the difficulty of implementation is greater. The efficient solution of the algebraic equations arising from pseudospectral collocation generally require the use

of sophisticated iterative methods. Additionally, the exact solution itself should be smooth on the computational domain in order that exponential convergence is attained. Finally, and perhaps most importantly, for problems of dimension greater than unity the computational domain must be sufficiently simple that it can be mapped to  $\mathbb{I}^d$  or be decomposed into sub-domains that can each be mapped to  $\mathbb{I}^d$  (*e.g.*, an L-shaped region can be decomposed into two regions, each of which can be mapped to  $\mathbb{I}^2$ ).

We have not here investigated the application of pseudospectral collocation techniques to evolution problems. Pseudospectral collocation methods have been used to solve problems in other fields (*e.g.*, fluid dynamics) with great success [2,15]. Our own experience in applying these techniques to evolution problems in numerical relativity shows promise, but is not yet complete.

### ACKNOWLEDGMENTS

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### APPENDIX A: SOLVING THE PSEUDOSPECTRAL COLLOCATION EQUATIONS

In this appendix we describe one method of solving the nonlinear equations that arise from applying a PSC method to a nonlinear elliptic system of equations

$$L(u) = f \quad \text{on } \mathcal{D}, \quad (\text{A1a})$$

$$S(u) = g \quad \text{on } \partial\mathcal{D}. \quad (\text{A1b})$$

Choosing an expansion basis and corresponding collocation points, the PSC solution of these equations is fully characterized by the values of  $u_N$  at the collocation points  $x_n$ : from these the coefficients of the expansion and all the derivatives of the approximate solution can be determined. Write the values of the approximate solution  $u_N$  at the collocation points  $x_n$  as a vector  $\mathbf{U}$ ,

$$\mathbf{U}_n = u_N(x_n). \quad (\text{A2})$$

Corresponding to the approximate solution  $u_N$  is a residual  $R_N$  on  $\mathcal{D}$  and  $r_N$  on  $\partial\mathcal{D}$ :

$$R_N = L(u_N) - f \quad \text{on } \mathcal{D}, \quad (\text{A3a})$$

$$r_N = S(u_N) - g \quad \text{on } \partial\mathcal{D}. \quad (\text{A3b})$$

The residual vanishes everywhere for the exact solution  $u$ . Write the values of the residual at the collocation points  $x_n$  as a vector  $\mathbf{R}$ ,

$$\mathbf{R}_n = \begin{cases} R_N(x_n) & x_n \text{ on } \mathcal{D} \\ r_N(x_n) & x_n \text{ on } \partial\mathcal{D}. \end{cases} \quad (\text{A4})$$

The PSC solution  $\mathbf{U}$  satisfies the algebraic equations

$$\mathbf{R}[\mathbf{U}] = 0. \quad (\text{A5})$$

Before describing how to solve equation A5 for a nonlinear system (*i.e.*, nonlinear  $L$  or  $S$ ) we describe the method of solution for a linear system.

When the system of differential equations A1 is linear so is the system of algebraic equations A5. In this case we can write

$$\mathbf{A}\mathbf{U} = \mathbf{F}, \quad (\text{A6})$$

where  $\mathbf{\Lambda}$  is a matrix and  $\mathbf{F}$  is a vector whose components take on the values of  $f$  and  $g$  evaluated at the collocation points in the domain  $\mathcal{D}$  and its boundary  $\partial\mathcal{D}$ . In PSC the matrix  $\mathbf{\Lambda}$  is typically full. Direct solution methods require  $\mathcal{O}(N^3)$  operations for such systems; for efficiency such systems are generally solved by iterative methods, which typically requires many fewer operations to find an accurate solution.

A simple and effective iterative method for solving equation A6 is Richardson's iteration. Suppose we have a guess  $\mathbf{V}^{(i)}$  to the solution  $\mathbf{U}$  of equation A6. A better approximation to  $\mathbf{U}$  is  $\mathbf{V}^{(i+1)}$  given by

$$\mathbf{V}^{(i+1)} = \mathbf{V}^{(i)} - \omega \mathbf{R}^{(i)}, \quad (\text{A7})$$

where the residual  $\mathbf{R}^{(i)}$  vector is given by

$$\mathbf{R}^{(i)} = \mathbf{\Lambda} \mathbf{V}^{(i)} - \mathbf{F}, \quad (\text{A8})$$

and  $\omega$  is a relaxation parameter, which must be determined. The optimal value of  $\omega$  and the rate of convergence of the iterations depend upon the eigenvalues of  $\mathbf{\Lambda}$ . For Richardson's iteration the optimal  $\omega$  is

$$\omega_{\text{opt}} = \frac{2}{\lambda_{\text{max}} + \lambda_{\text{min}}}, \quad (\text{A9})$$

where  $\lambda_{\text{max}}$  and  $\lambda_{\text{min}}$  are the largest and smallest eigenvalues of  $\mathbf{\Lambda}$ . This choice minimizes the spectral radius  $\rho$ ,

$$\rho = \frac{\lambda_{\text{max}} - \lambda_{\text{min}}}{\lambda_{\text{max}} + \lambda_{\text{min}}}, \quad (\text{A10})$$

of the iteration matrix,  $G = I - \omega \mathbf{\Lambda}$ . The convergence rate of the iteration is [2]

$$\mathcal{R} = -\ln \rho. \quad (\text{A11})$$

The reciprocal of  $\mathcal{R}$  measures the number of iterations required to reduce the error by a factor of  $e$ .

Richardson's iteration is, by itself, not necessarily more efficient than a direct solution method. Consider, for example, the second-order differential equation

$$\frac{d^2 u}{dx^2} = f(x) \quad x \in (-1, 1), \quad (\text{A12a})$$

$$u(-1) = u(1) = 0 \quad (\text{A12b})$$

(cf. also section IV). A PSC solution with a Chebyshev expansion basis leads to an operator  $\mathbf{\Lambda}$  with a spectral condition number  $\lambda_{\text{max}}/\lambda_{\text{min}}$  that is  $\mathcal{O}(N^2)$ . This gives a rate of convergence  $\mathcal{R} \sim \mathcal{O}(N^{-2})$ ; correspondingly,  $\mathcal{O}(N^2)$  iterations are required to obtain a reasonable solution. Since each iteration requires  $\mathcal{O}(N \ln N)$  operations (*i.e.*, it is asymptotically dominated by the cost of evaluating the derivatives  $d^2 u/dx^2$  given the  $N+1$   $u_N(x_n)$ ) the total cost of obtaining a solution  $\mathbf{U}$  is  $\mathcal{O}(N^3 \ln N)$ , which is slightly *more* expensive than a direct solution.

We can speed the convergence of Richardson's iteration by solving an equivalent problem whose spectral condition number is better behaved. Introduce the *preconditioning* matrix  $\mathbf{H}$  and consider the equivalent system

$$\mathbf{H}^{-1} \mathbf{\Lambda} \mathbf{U} = \mathbf{H}^{-1} \mathbf{F}. \quad (\text{A13})$$

Now given an approximation  $\mathbf{V}^{(i)}$  to  $\mathbf{U}$ , a better approximation  $\mathbf{V}^{(i+1)}$  is given by

$$\mathbf{V}^{(i+1)} = \mathbf{V}^{(i)} - \omega' \mathbf{H}^{-1} \mathbf{R}^{(i)}, \quad (\text{A14})$$

where  $\mathbf{R}^{(i)}$  is given as before and  $\omega'$  is related to the eigenvalues of the linear operator  $\mathbf{H}^{-1} \mathbf{\Lambda}$ .

In practice we never actually invert the preconditioning matrix  $\mathbf{H}$ ; instead we solve

$$\mathbf{H} \left( \mathbf{V}^{(i+1)} - \mathbf{V}^{(i)} \right) = -\omega' \mathbf{R}^{(i)}, \quad (\text{A15})$$

for successive approximations. In order that this equation for successive approximations should converge rapidly we require a preconditioning matrix  $\mathbf{H}$  such that

- equation A15 is inexpensive to solve, and
- the spectral condition number  $\kappa'$  of  $\mathbf{H}^{-1} \mathbf{\Lambda}$  is close to unity.

If  $\mathbf{H}^{-1}$  is a good approximation of  $\mathbf{\Lambda}^{-1}$  then the second condition will be satisfied; consequently, we look for approximations to  $\mathbf{\Lambda}$  for which equation A15 is inexpensive to solve.

The operator  $\mathbf{\Lambda}$  arises from a system of differential equations. For one-dimensional problems a low-order FD approximation to this operator (with grid points coincident with the collocation points) gives rise to a banded system with a small number of bands close to the main diagonal. When this FD operator is used as the preconditioner the system of equations A15 can be solved efficiently using direct methods.<sup>§§</sup>

For instance, in the example considered here (eq. A12) we can set  $\mathbf{H}$  to be the second-order accurate FD operator corresponding to  $L$ . The eigenvalues of the preconditioned operator  $\mathbf{H}^{-1} \mathbf{\Lambda}$  are all in the range  $1 \leq \lambda_p^{PC} \leq \pi^2/4$ : *i.e.*, the spectral condition number is independent of  $N$ . In this case the optimal relaxation parameter is

$$\omega'_{\text{opt}} \approx \frac{4}{7}, \quad (\text{A16})$$

and each iteration reduces the residual by a factor of approximately 7/3 (independent of  $N$ ) [14]. The asymptotic cost of finding a solution is thus proportional to the cost of evaluating the residual,  $\mathcal{O}(N \ln N)$ , which is

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<sup>§§</sup>For more details on the use of FD operators as preconditioners for spectral problems see [14].

much more rapid than solution via a direct method or Richardson's iteration without a preconditioner.

For higher dimensional problems the FD preconditioner still leads to a banded system with a small number of non-zero bands; however, some of those bands are found far from the main diagonal and equation A15 can no longer be solved efficiently using direct methods. If  $N$  becomes so large that the cost of solving these equations with the FD preconditioner is too great, then the equations for the successive approximations can themselves be solved iteratively, other preconditioners can be explored (cf. [1,2,16]), or the original equations can be solved using another iterative technique, such as multigrid [5]. For the problems considered in this paper  $N$  never became so large that a direct solution of equation A15 with the FD preconditioner was problematic.

If the equations A1 are nonlinear, the algebraic equations satisfied by  $\mathbf{U}$  are similarly nonlinear. Write the nonlinear equations as

$$\mathcal{L}(\mathbf{U}) = \mathbf{F}, \quad (\text{A17})$$

where  $\mathcal{L}$  is a nonlinear function of  $\mathbf{U}$ . In order to solve this nonlinear system of equations, we apply Newton's iteration [1, sec. 12.13 and appendices C and D]. For equation A5, Newton's iteration is

$$\mathbf{\Lambda}_{\mathbf{V}^{(i)}}(\mathbf{V}^{(i+1)} - \mathbf{V}^{(i)}) = -\mathbf{R}^{(i)}, \quad (\text{A18})$$

where  $\mathbf{\Lambda}_{\mathbf{V}^{(i)}}$  is the *linear* operator that arises from linearizing  $\mathbf{\Lambda}$  about  $\mathbf{V}^{(i)}$  and  $\mathbf{R}^{(i)}$  is the *nonlinear* residual given by

$$\mathbf{R}^{(i)} = \mathcal{L}(\mathbf{U}) - \mathbf{F}. \quad (\text{A19})$$

Equation A18 is a linear system to be solved at each step of Newton's iteration. In the same way as before we can introduce a preconditioner, in which case we have the nonlinear Richardson's iteration

$$\mathbf{H}(\mathbf{V}^{(i+1)} - \mathbf{V}^{(i)}) = -\omega' \mathbf{R}^{(i)}. \quad (\text{A20})$$

Here  $\mathbf{H}$  is any suitable preconditioning matrix for  $\mathbf{\Lambda}_{\mathbf{V}^{(i)}}$ . For the problems solved in section V we used as a preconditioning matrix a second-order accurate FD operator corresponding to the derivative terms of  $\mathcal{L}$  *ignoring* the nonlinear terms. (Equivalently we could have used the FD operator corresponding to the linearized operator, but for the problems we examined this was not necessary.)

As a quick demonstration, consider the example problem

$$\frac{d^2 u}{dx^2} - e^x[(1 - \pi^2) \sin(\pi x) + 2\pi \cos(\pi x)] = 0, \quad (\text{A21})$$

$$u(-1) = u(1) = 0. \quad (\text{A22})$$

We have evaluated approximate solutions to this problem using a second-order accurate FD approximation and a

TABLE I. The values of the absolute error  $\Delta u_{PSC}$  of a PSC calculation, as well as the absolute error of a second-order FD calculation  $\Delta u_{FD}$  for several values of  $N$  for the example problem (equation A21). For  $N > 16$ , the PSC solution is contaminated with roundoff errors.

$N$	$\Delta u_{PSC}$	$\Delta u_{FD}$
4	$1.7 \times 10^{-1}$	$2.5 \times 10^{-1}$
8	$3.2 \times 10^{-4}$	$5.4 \times 10^{-2}$
16	$6.9 \times 10^{-10}$	$1.3 \times 10^{-2}$
32	-	$3.3 \times 10^{-3}$
64	-	$8.2 \times 10^{-4}$
128	-	$2.1 \times 10^{-4}$

PSC approximation on a Chebyshev basis. For this problem we know the exact solution,

$$u(x) = e^x \sin(\pi x). \quad (\text{A23})$$

Table I lists  $\Delta u_{PSC}$  and  $\Delta u_{FD}$  (cf. 5.10) for increasing  $N$  (number of grid points for the FD approximation, basis dimension for the PSC approximation). The rapid convergence of PSC is apparent. The second-order FD solution requires 128 points to equal the moderate accuracy of an eighth-order PSC solution. In order to match the high accuracy of the 16th-order PSC solution would require a second-order FD solution with  $6.5 \times 10^4$  points.